

An infra-red band-system of calcium oxide

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With 11 figures in the text

Abstract

This investigation gives vibrational and rotational analyses of a $^1\Sigma-^1\Sigma$ band-system of calcium oxide. The analysed part of the spectrum contains five sequences at 7308, 7715, 8153, 8652 and 9229 Å. Sixteen bands have been analysed, namely, the 6,3, 5,2, 5,3, 4,1, 4,2, 3,0, 3,1, 3,2, 2,0, 2,1, 2,3, 1,0, 1,1, 1,2, 0,0 and 0,1 bands. The constants derived are:

$$\begin{aligned} B_v'' &= 0.4444_7 - 0.0033_5 (v + \tfrac{1}{2}) + 0.00000_5 (v + \tfrac{1}{2})^2 & B_v' &= 0.4063 - 0.0014_1 (v + \tfrac{1}{2}) \\ D_v'' &= [0.657 + 0.03 (v + \tfrac{1}{2})] \times 10^{-6} & D_v' &= 0.54 \times 10^{-6} \\ r_e'' &= 1.822 \times 10^{-8} \text{ cm} & r_e' &= 1.906 \times 10^{-8} \text{ cm} \\ \omega_e'' &= 732.1_1 & \omega_e' &\sim 716 \\ x_e'' \omega_e'' &= 4.8_1 & x_e' \omega_e' &\sim 1.6 \end{aligned}$$

$$\nu_{0,0} = 11548.8$$

In the upper state some thirty perturbations have been found. They can be explained as interactions with six electronic states or substates. As the lowest level $v' = 0$ in the upper state is perturbed, the absolute v -numbering of the perturbing states cannot be obtained. Four of the perturbing states — called X , Y , Z and Q — have about the same B and ω -values — $B \sim 0.33$ and $\omega \sim 500$. The other two perturbing states — called A and B — have B -values of about 0.38 and $\omega \sim 600$.

In the 0,0 band at $J \sim 53$ the two states A and Z perturb the upper Σ -level Σ^* . In this part of the spectrum the 0,0 band has three R -lines and three P -lines. Formulas for the determination of B and C -values for three interacting states are given. The general case with n interacting terms is also treated.

§ 1. Introduction

The addition of calcium salts to flames or arcs gives a lot of bands and band-systems, most of which are attributed to CaO. These bands appear in the infra-red, extreme red, orange and green, and in arcs in the blue, violet and near ultra-violet also. MAHANTI (1932) and KING (1908) considered that

the green and orange bands belong to Ca_2 , on the other hand some other authors ascribe them to CaO . In this paper we shall not discuss this point, but only underline how little is known with certainty about the CaO -spectrum.

Several bands have been arranged into head-formulas. Thus MAHANTI (1932) and BRODERSEN (1936) gave such vibrational equations for the blue bands, MAHANTI for some ultra-violet ones too. MEGGERS (1933) measured infra-red bands from about 7000 Å to 10500 Å and tried to arrange them into two systems. BRODERSEN then remeasured some of the infra-red bands and altered MEGGERS' analysis. BRODERSEN gave some rotational analyses of these bands and of some blue bands. He also tried to arrange ten band-systems of CaO into a term scheme, representating seven electronic states. LEJEUNE and ROSEN (1945) have also tried to build up a term scheme from their own measurements and the papers mentioned above. We shall, however, only discuss in detail here the infra-red bands between 7000—9400 Å. On the other hand we may mention that we also have photographed some ultra-violet and blue bands in a rather high dispersion (about 1.2 Å/mm in a Wood's 21 ft concave grating) and a preliminary study has shown that certain measurements published in some of the papers mentioned above are somewhat doubtful.

In his first paper (1932) BRODERSEN gave vibrational and rotational analyses of bands between 6600 and 8700 Å, which he attributed to a $^1\Sigma-^1\Sigma$ transition. He made rotational analyses on the bands he termed 0,0 (7308 Å), 1,1 (7318 Å) and 1,4 (8652 Å). In the 8652-band he found a perturbation at about $J \sim 53$ in the lower level. He mentions, however, some drawbacks in his vibrational scheme. Thus the bands with $v' = 1$ are more intense than those with $v' = 0$, and no bands were found with v' greater than 3. The last phenomenon he explains as the effect of a possible predissociation or that bands with $v' > 3$ are hidden in the multitude of lines. The perturbation mentioned is not analysed in any other band with $v'' = 4$. An examination of the rotational constants he calculated shows that the B -values do not agree very well.

In his next paper (1936) BRODERSEN gave rotational analyses of some blue bands and drew up the term scheme already mentioned. The results of his analyses of the red bands did not agree with this scheme. He was therefore obliged to alter his previous analyses. This he did in the following way. All bands with $v' = 0$ he now considered as belonging to another system. In this way he escaped the disadvantage of the bands $v' = 0$ being weaker than those with $v' = 1$. Thus the bands which previously had $v' = 1$ now have $v' = 0$. But this is not enough, the v'' -numbers are increased by one unit and a new (apparently unregistered) band at 6625 Å (15090 cm^{-1}) becomes the 0,0 band. The 8652-band, which in the first paper was considered as the 1,4 band, ought now to be the 0,5 band. BRODERSEN, however, transfers this band to a new system. Of the three bands, which were formerly rotationally analysed only the band at 7318 Å remains in the now almost unrecognizable old system. But the rotational analysis of even the 7318-band is altered. The J -numbering is new. The same is true of the 7308-band, which is now placed in yet another system (together with the former $v' = 0$ bands). The arrangement is confusing. The whole term scheme seems to us to be very unreliable.

In order to interpret the complicated CaO -spectrum the best thing seemed to us to start with the infra-red bands treated by BRODERSEN. The spectrograms he published (1932) led us to believe that it should be possible to make

trustworthy rotational analyses of some bands (especially of the 8652-band), particularly as we could use spectroscopic instruments of higher dispersion and resolution power.

This investigation gives complete analyses, both vibrational and rotational, of the infra-red $^1\Sigma-^1\Sigma$ system situated between 7300 and 9400 Å. The analyses were difficult to carry out due to a lot of perturbations, which totally destroy the positions of the bands in the sequences. BRODERSEN's analyses of this part of the CaO-spectrum are completely wrong.

§ 2. Experimental

Spectrograms in the region from 7000 Å to 9000 Å were taken in a first order of a 21-ft Wood concave grating (165000 lines) having a dispersion of about 1.1 Å/mm. Spectrograms were also taken in both a first (8800—11000 Å) and a second (9050—10000 Å) order of a Rowland plane grating (47000 lines) having a dispersion of about 10 Å/mm and 4.5 Å/mm in the orders used.

We used two different sources of light. One was an arc burning in air between carbon electrodes, the upper negative, the lower positive. The current was 4—7 amp. taken from a 440 volts D. C. output. The lower electrode was filled with fused calcium chloride. (The carbon cylinder was filled with salt while a large alternating current of about 200 amp. was lead through the cylinder. The method was employed by BRODERSEN.) The other source of light was an arc burning in air between pure calcium electrodes. The current was about 4 amp. from a 440 volts D. C. output. The spectrum obtained from the second source of light was a little more intense than that obtained from the first. The first source was used for the spectrograms taken in the Wood concave grating. The exposure time was 7 hours. The second source was used for the plane grating spectrograms. The exposure time was then about 2 hours. The plates used were Eastman Kodak IL, IM, IN and IZ, which were hypersensitised with ammonia before exposure. For comparison, iron lines were used for the concave grating exposures, and barium, calcium and iron lines for those with the plane grating. M. I. T. tables (1939) were used.

§ 3. Structure of the bands

On a plate taken in a spectrograph with a relatively small dispersion five clear sequences — shaded towards the red — appear in the CaO spectrum at 7308, 7715, 8153, 8652 and 9229 Å. Towards longer wavelengths the spectrum becomes more complicated. These five sequences are very intense. Fig. 1 a shows the five sequences, taken in a large quartz spectrograph. (A 30° prism of 10 × 15 cm² aperture, focal length about 4 m, diameter of the lens 12 cm, dispersion of 30 Å/mm at 8000 Å.) Fig. 1 b shows the sequence at 9200 Å and a lot of bands above this sequence. The spectrogram is taken in a first order of the plane grating.

This investigation shows that the five sequences belong to a single band-system. The transition is a $^1\Sigma-^1\Sigma$. The sequence $\Delta v = 0$ is the one at 8652 Å, $\Delta v = -1$ that at 9229 Å, $\Delta v = +1$ that at 8153, and so on. Some of the bands above 9229 Å (see Fig. 1 b) belong to this band-system, most of them to other transitions.

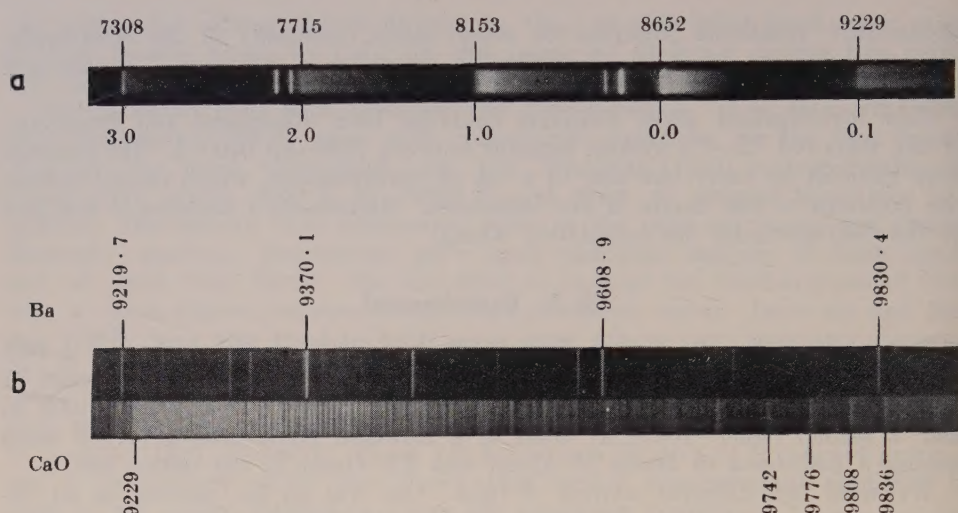


Fig. 1. Spectrograms of the infra-red CaO bands, a) taken in a quartz spectrograph, b) the $\Delta v = -1$ sequence taken in a first order of a plane grating. Some bands situated towards higher wave-lengths appear. They do not belong to the system investigated.

Perturbations have been found in all the bands. The upper levels are perturbed, the lower ones unperturbed. Some of the perturbations are so strong that they completely destroy the positions of the bands in the sequences. Thus a strong perturbation at $J \sim 18$ in the level $v' = 2$ effects two heads for bands with $v' = 2$ as upper level. Table 1 gives the band-heads and the band-intensities. The intensities have been estimated by comparing the intensities of the rotational lines. Comparing the band-heads gives an incorrect result. At about 9215 Å a weak band-head is situated, which does not belong to the system.

Table 2 gives the calculated band-origins. In § 7 the methods by which these were determined are described.

We started with the 8652-band. BRODERSEN's analysis of this band seemed to us to be rather sensible, as the combination differences for one of the levels

Table 1

Band-heads and estimated intensities (in brackets) of the infra-red CaO bands

6				not observed (3)
5				~ 7724 (2)
4			~ 7326 (7)	
3		7318.46 (7)	7721.15 (6)	
2	7308.31 (1)	7715.54 (8)	~ 8164.7 (1)	
1	{ ~ 7687.8 (8)	{ not measured (7)		{ not observed (4)
0	7712.25 (8)	8167.30		{ not observed
	8153.08 (9)	not observed (0)	~ 9230 (8)	
	8652.20 (10)	9229 (8)		
↑ v'				
$v'' \rightarrow$	0	1	2	3

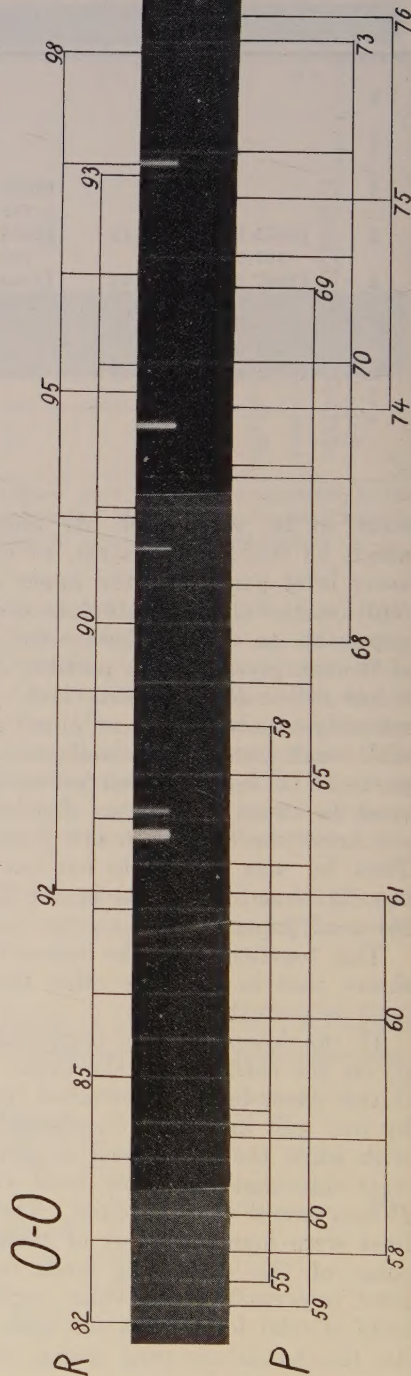
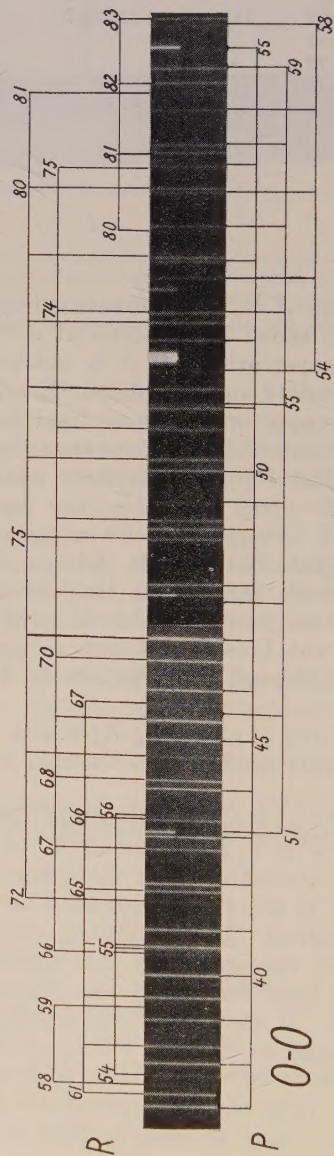
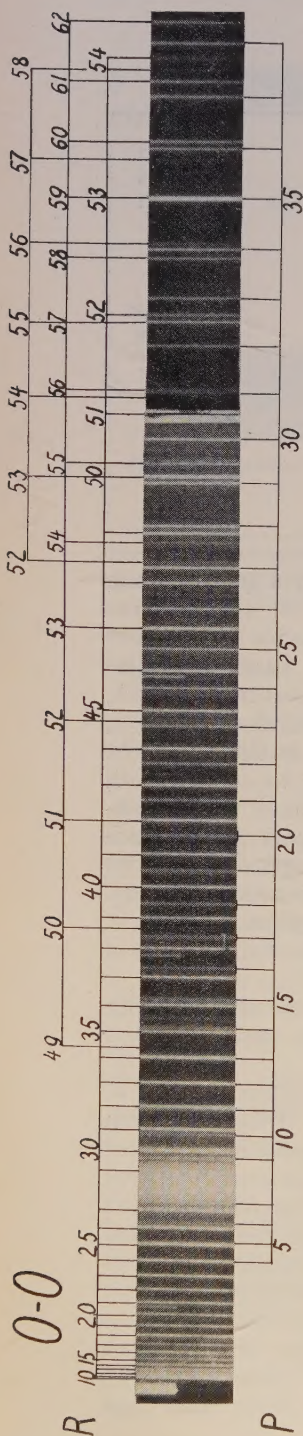
Table 2
Band-origins

6						13634.23
						695.36
5				13642.06	703.19	12938.87
				698.46		
4			13655.59	712.67	12942.92	
			702.51		703.22	
3	13675.18	722.10	12953.08	713.38	12239.70	
	707.92		708.31			
2	12967.26	722.49	12244.77			10829.53
	706.75		706.83			
1	12260.51	722.57	11537.94	712.88	10825.06	
	711.67		712.07			
0	11548.84	722.97	10825.87			
↑ v'						
$v'' \rightarrow$	0		1		2	3

seem to be very good. At about $J = 53$ BRODERSEN found a perturbation, which he could not analyse, so he ended his analysis at $J = 54$, assuming the lower level perturbed, the upper unperturbed. If it is not possible to recognize $R(0)$ and $P(1)$ with absolute certainty in an isolated ${}^1\Sigma$ — ${}^1\Sigma$ band, it is also impossible to decide whether the upper or the lower level is perturbed, which, of course, gives us two possible J -numberings. BRODERSEN published, however, a line called $R(0)$ in this band. But $R(0)$ is extremely weak in this band (the intensity-maximum lies at about $J = 60!$) and it is very easy to confuse $R(0)$ with weak lines in the background. There are a lot of such lines in the background. It is also remarkable, that BRODERSEN did not report $R(1)$, which must be twice as intense. Further it seems to us that BRODERSEN himself did not trust the lines with low J -values which he himself gave as rotational lines. Thus he was obliged to cut out the lines in his first paper given as $R(0)$ in the 7308-band and $R(1)$ in the 7318-band when he altered the J -numbering in his next paper.

This together with the impossibility of obtaining $R(0)$ with sufficient intensity shows that in this case other factors must decide whether the upper or lower level is perturbed.

If the lower level is perturbed, $\Delta^2 F'(J)$ must change continuously with J , if, on the other hand, the upper level is perturbed $\Delta^2 F''(J)$. This means that if the upper level is perturbed the J -numbering of the R -lines must be decreased by one unit and the J -numbering of the P -lines increased by one unit compared with when the lower level is perturbed. After analysing only the 8652-band we were sure that the upper level was the perturbed one, although the first R and P -lines could not be found. The band has about ten perturbations and extra lines were found at some of them. If we assume the upper level is perturbed some of the perturbing levels ought to have $B \sim 0.33$, if, however, the lower level is perturbed this value ought to be about 0.56. A B -value of the magnitude of 0.56 for CaO is too high. (For the calculations see § 5 Equ. 5 and 15.) As the bands are very strong it is easy to imagine that the lower state may



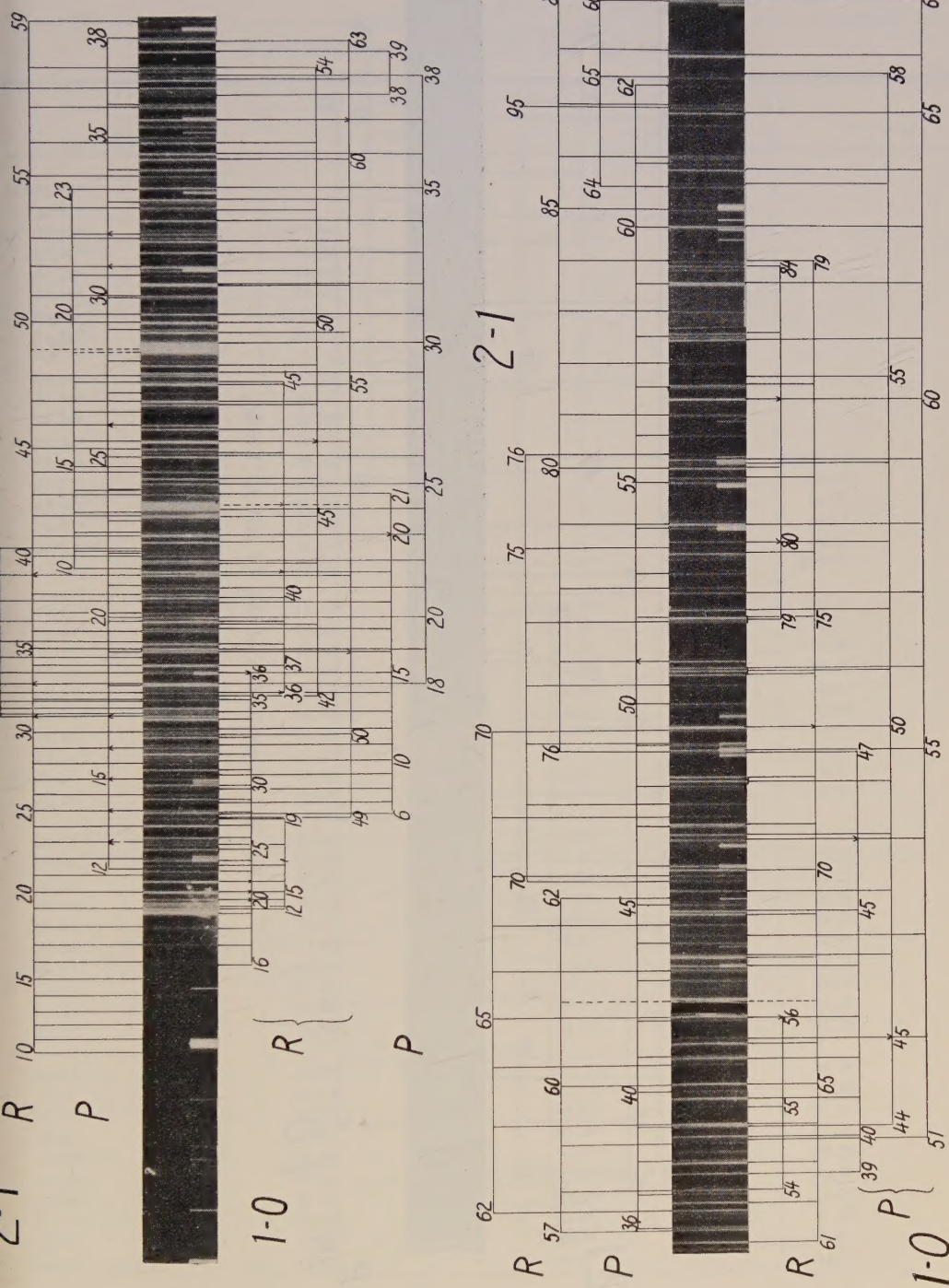


Fig. 3 a—b. Reproductions of the 1,0 and 2,1 bands.

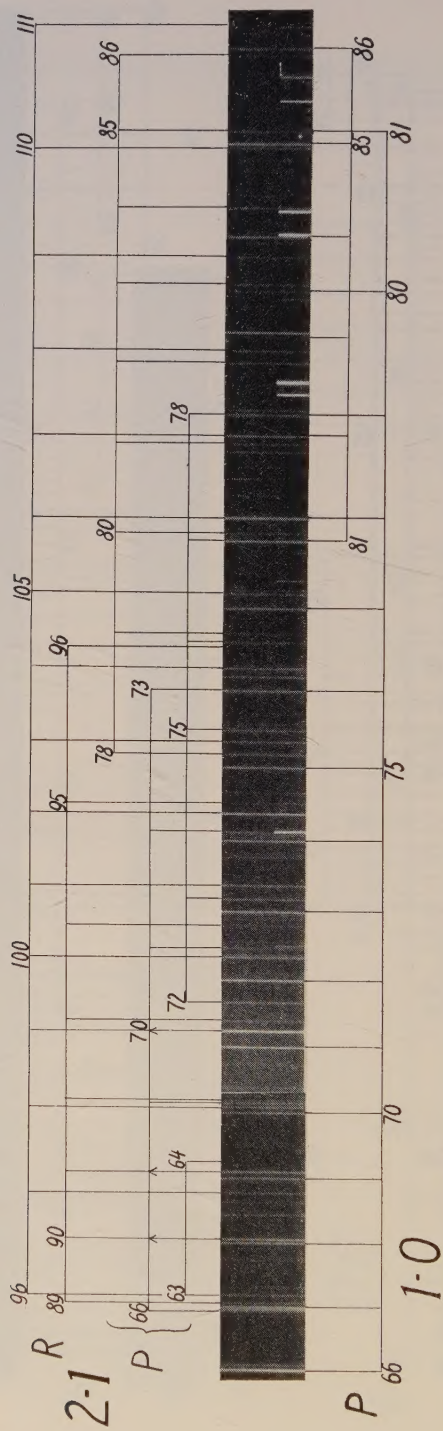


Fig. 3 c. Reproduction of the 1,0 and 2,1 bands.

Table 3

Wave-numbers for the 0,0 and 0,1 bands

0,0		0,1	
<i>R (J)</i>	<i>P (J)</i>	<i>R (J)</i>	<i>P (J)</i>
11552.82*			
53.31*			
53.69*	11546.68		
54.02*	45.29		
54.29*	43.88		
54.49*	42.47		
54.59*	Ca-line		
54.59*	39.39		
54.59*	37.78		
54.49*	36.05		
54.29*	34.20*		
54.02*	32.37		
53.69*	30.40		10808.6*
53.31*	28.36		06.8*
52.82*	26.25		04.7*
52.27*	24.09		02.6*
51.64	21.84		00.4*
50.96	19.51		798.2
50.14	17.14	10829.3*	96.0
49.37	14.68	28.4*	93.9*
48.48	12.18	27.4*	91.3*
47.52	09.58	26.8*	89.0
46.48	06.94	25.9*	86.4
45.39	04.21	25.1*	83.8*
44.24	01.44	24.1*	81.2
43.00	498.59	23.0*	78.5*
Ca-line	95.66	22.0*	75.8
40.29	92.66	20.7*	73.1*
38.91	89.61	19.4*	70.2*
37.40	86.46	18.3	67.2*
35.82	83.26	17.0*	64.2*
34.20*	80.00	15.5*	60.9*
32.44	76.67	13.9*	58.1*
30.68	73.20*	12.3*	54.9*
28.84	69.80	10.5*	51.7*
26.89	66.27	09.1*	48.3*
24.89	62.66	07.3*	45.2*
22.82	58.99	05.4	41.7*
20.66	55.26	03.7*	38.2*
18.41	51.41	01.7*	34.6*
16.08*	47.52	799.6*	31.0
13.67	43.52	97.5*	27.3*
11.15	39.46	95.2*	23.7*
08.50	35.30	92.9*	19.6*
05.72	31.04	90.4*	15.7*
02.76*	26.69	87.8*	11.8*
499.63	22.14	85.0*	07.6
96.18 11531.74	17.47	81.8*	03.3

M. HULTIN AND A. LAGERQVIST, *An infra-red band-system of calcium oxide*

Table 3 (cont.)

J	0,0				0,1			
	R (J)		P (J)		R (J)		P (J)	
50	11492.21*	11523.49	11412.58		10778.1*		10698.5*	
51	87.42	16.08*	07.40	11443.00	73.7		93.6	
52	81.16	09.19	01.68	33.12*	67.8*	10785.0*	88.3*	
53	73.20*	02.76*	395.13	23.67	60.2*	10789.9*	79.2*	82.2*
54	63.70	496.83	87.21	15.25	51.1	85.0*	74.5*	74.6*
55	53.12	91.34	77.53	07.07		79.2*	69.6*	65.4
56	41.81	86.25	66.30	399.41*		74.5*	64.2*	54.6
57		81.62	53.97	92.19		70.2*	59.0*	80.8
58		77.30	41.10*	85.42		66.2	53.7*	74.6*
59		73.20*		79.06		62.3*		58.4
60		69.33		73.02	59.0*		62.8	50.3
61		65.25		67.14	55.4*		57.3*	
62		61.23		61.60	51.7*		52.2	
63		57.13		55.82	48.3*		46.9*	
64		52.87		50.12	44.2*		41.7	
65		48.16		44.31	39.9		36.1	
66	453.50	42.14		38.33	745.7*	34.6*	30.7*	
67	44.60	32.31		31.94	37.3	25.0	24.7	
68	38.76		335.58	24.20	31.9*		17.3*	
69	33.65		24.98	12.62	27.3*		18.5	06.4
70	28.52		17.42		22.7*		11.6	
71	23.00		10.61		17.7		05.3	
72	16.80	449.05	03.79		11.8*	744.2*	599.0	
73	09.16	36.77	296.62		04.9*	31.9*	92.3	
74	399.41*	26.50	88.75	320.94	695.6*	22.7*	84.8	617.3*
75	87.47	18.35	79.38*	07.01	84.4*	15.0*	76.0	03.6*
76		11.67	67.90	295.02			65.0	592.0*
77		05.76	54.50*	85.25			52.0*	82.9
78		00.23		76.84				
79		394.80		69.26				
80	392.78	89.07		62.06				
81	86.10	81.22		54.96				
82	80.28		251.32	47.56				
83	74.89		42.93	38.06				
84	69.54		35.45					
85	64.14		28.41					
86	58.63		21.41					
87	53.06		14.35					
88	47.24		07.24					
89	41.10		199.25					
90	34.47		92.49					
91	26.93		84.72					
92	17.64	352.10*	76.45					
93	05.37	39.26	67.30					
94		27.53	56.4	190.66				
95		19.46	42.4	76.06				
96		11.79		62.96				
97		04.63		53.35				
98		297.37		44.03				
99		88.55		35.36				

Table 3 [cont.]

J	0,0		0,1	
	$R(J)$	$P(J)$	$R(J)$	$P(J)$
100		11126.3		
101	11281.43	15.8		
102	74.04			
103	66.31	11105.6		
104	56.78 11279.38*	096.6		
105	64.25	87.4		
106	54.50*	76.5		098.8
107	46.76			82.3
108	39.67			70.8
109	32.8			61.4
110	26.0			52.9
111	19.1			44.3
112	12.3			35.9
113	05.3			27.5
114	198.1			19.2
115	90.7*			10.5
116	82.7			01.8
117	73.8			10992.2
118				82.9
119				72.4

probably be the ground state and for this reason is unperturbed. We shall only point out that it is at first more natural to assume that the upper levels are perturbed.

Since the 1,0 (8153) and 0,1 (9229) bands had been analysed, our assumption was confirmed.

In the 0,0 band (8652) two electronic states perturb the upper level $v' = 0$ at about $J \sim 53$. At this perturbation three R and P -lines have been found for every J -value. The lines given as $R(53)$, $R(54)$, $P(53)$ and $P(54)$ by BRODERSEN in this region are all incorrect.

BRODERSEN's analysis reminds one of that by MAHLA for SrO. MAHLA also confused the upper and the lower states and assumed that the lower state was the perturbed one. (See ALMKVIST and LAGERQVIST, 1949.)

The appearance of the structure of the 0,0, 1,0 and 2,1 bands is shown in Figs. 2 and 3. The structure is open as the bands lie on a wide Condon parabola. The heads are formed by lines of low J -values, commonly $R(7)$ to $R(10)$. Sixteen bands in all have been analysed.

The wave-numbers of the lines are given in Tables 3—8, where overlapped lines are indicated with an asterisk. Where the lines of the 0,0 and 1,1 band coincide, asterisks have been used for the 1,1 band lines but not for the 0,0 lines, due to the fact that the latter are very much stronger than the former. The wave-numbers of the lines taken in the concave grating are given to two decimalplaces, lines taken in the plane grating to one. The second order plane grating lines are used above 9050 Å, the first order lines only between 9000 and 9050 Å. In all the bands in which perturbations have been found, two columns are given for both R - and P -lines, one for each of the interacting levels. In the 0,0 and 0,1 bands three columns must be used for the perturba-

Table 4

Wave-numbers for the 1,0, 1,1 and 1,2 bands

J	1,0		1,1		1,2	
	R (J)	P (J)	R (J)	P (J)	R (J)	P (J)
4	12260.89					
5	61.30					
6	61.61	12251.21				
7	61.87*	49.81				
8	61.94*	48.35				
9	61.94*	46.81				
10	61.94*	45.18				
11	61.87*	43.46				
12	61.61	41.64				
13	61.09*	39.68				
14	60.52	37.66*				
15	59.70*	35.45*				
16	58.55* 12267.67	33.08*			10834.3	
17	56.77 65.49	30.50			32.3*	
18	54.47 63.63	27.51 12236.61*			30.8*	10803.3
19	51.61* 62.21	24.11* 32.76*			29.5*	000
20	61.09*	20.01 29.24		11508.22	28.4*	796.8
21	59.70*	15.31* 25.96	11538.91*	05.09	27.4*	93.1
22	58.55*	22.87	37.78*	02.13	26.8*	91.1
23	57.42	20.01*	36.95	499.34	25.9*	88.8
24	56.24	17.02	35.82*	96.83*	25.1*	85.1
25	54.99	14.12	34.68	93.84	24.1*	83.1
26	53.71	11.18*	33.62	91.08	23.0*	80.1
27	52.40*	08.17	32.50*		22.0*	78.8
28	50.94	05.10*	31.27	85.39	20.7*	75.1
29	49.43	02.02	29.73	82.55	19.9	72.1
30	47.83	198.83	28.36*	79.50	18.7*	69.1
31	46.18	95.57	26.89*	76.28*	17.4	66.1
32	44.46	92.22	25.58	73.20*	16.1*	64.1
33	42.59	88.81	24.09*	70.20	14.8	60.1
34	40.59	85.31	22.18	66.78	13.3	58.1
35	38.41*	81.70	20.02		12.0	54.1
36	237.66* 35.45*	77.96	11519.76		10.5*	51.1
37	34.54	74.19*			10808.6*	48.1
38	32.19	171.54 69.35	14.68*		06.8*	
39	29.71	66.68	12.55	11449.43	04.7*	10741.7*
40	27.04	62.57	10.09	45.59	02.6*	38.2*
41	24.11*	58.42	07.44	41.81	00.4*	34.6*
42	20.76 238.05	53.95	04.21*	37.53	797.5*	30.7*
43	Na-line 30.01	49.38*	00.48	33.12*	93.9*	26.6
44	10.76 23.13	44.14 161.40*	495.01	28.11	88.4*	22.1*
45	02.93 17.93	38.22 51.72*	502.45	22.73	81.8*	796.5*
46	13.60	30.60* 43.03	498.18*	15.25	92.0*	16.9*
47	09.47*	21.23*	36.04		89.4	09.8*
48	05.50	30.03	90.94	421.23	85.8*	01.1*
49	251.61* 01.21	24.26	537.40* 86.80*	10.07	32.3*	82.2

Table 4 (cont.)

1,0				1,1				1,2			
<i>R (J)</i>		<i>P (J)</i>		<i>R (J)</i>		<i>P (J)</i>		<i>R (J)</i>		<i>P (J)</i>	
2242.25	12196.48*	12118.47	11528.30*	11482.55*	11460.87	11404.56	10723.5*	78.1*	10700.3		
33.08*	90.86	12162.95	12.43	19.51*	77.30*	49.43	398.85	15.5*	73.1*	10745.2*	694.9
24.51*	84.18*	51.72*	05.93	11.15*	70.89	38.49	92.78	07.3*	67.2*	34.6*	89.1
Na-line	76.76*	40.88	098.63	03.77	63.70*	28.11*	85.75	00.4*	60.2*	24.5*	82.2
09.47*	68.48*	30.60*	90.20	497.07	56.02	18.10	77.53	693.9		15.0*	74.4
03.21	59.32	20.88	80.99	91.34*		08.87		88.4*		06.2	66.3
197.58	49.38*	12.10	70.84*	85.85		00.23*		83.8*		698.5*	57.3
92.44		04.08	60.16	81.16*		392.78*		79.2*		91.0	46.9
87.61		096.76*	48.59	76.67*		85.75*		75.3		84.4*	
83.00		89.84		72.29		79.06*		71.5*		78.3	
78.56		083.35		68.38		73.02*		67.8*		72.6	
74.19*		77.02		64.46*				64.2*		67.1*	
69.86		70.84*		60.46				60.9*		61.7	
65.52		64.74		56.58				57.3*		56.5	
61.17*		58.72		52.42				53.7*		51.3	
56.90*		52.66						50.2*		46.2	
52.34		46.61						46.8		41.1	
47.81*		40.52						43.2		36.1*	
43.26		34.40						39.5*		30.7*	
38.58		28.19						35.7		25.4	
33.81		21.91						31.9*		20.1	
28.90		15.57						28.0*		14.6	
23.81		09.09						23.7*		09.2	
18.47*		02.47						19.6*		03.6	
12.84		11995.72						15.0*		597.8	
06.74*		88.72						09.8*		92.0*	
099.89		81.40						04.1		85.5	
91.82		73.60						597.0*		78.8	
81.85		65.01						88.3*		71.4	
68.54	107.03	55.38*						75.9		62.6	
	098.63	43.71								52.0*	
	90.78*	28.70	11967.21*							38.3	
	83.35*		57.37								
	76.35		47.58								
	69.05		38.57								
			29.86								
			20.94								

Table 5
Wave-numbers for the 2,0, 2,1 and 2,3 bands

J	2,0		2,1		2,3	
	R (J)	P (J)	R (J)	P (J)	R (J)	P (J)
8			12240.50*	12279.70		
9	12962.35	13000.67	40.24*	78.59		
10	61.88	12999.42	39.92*	77.38	12223.79	12262.91
11	61.34*	97.95	39.37*	75.99	21.78	60.13
12	60.53	96.36	38.60	74.43	19.67	57.08
13	59.62	94.64	37.66*	72.82	17.37*	54.18
14	58.34	92.82	36.60*	72.42	14.76*	50.67
15	57.05*	90.93	34.11*	69.05*	12.28	47.23
16	54.98*	88.89	30.90*	65.26*	9.38*	43.81
17	53.18*	86.73	27.76	61.64	6.34	40.24
18	51.04*	K-line	24.12*	57.93	02.93*	36.79
19		82.75	20.51*	54.12	199.38	33.08
20		80.73	16.51*	50.32	24.51*	29.24
21		78.73		46.52*	21.49	25.64
22		76.73		42.74		21.99
23		74.77		38.91*		18.36
24		72.87		35.13*		14.76
25		70.95		31.45*		11.18*
26		69.05*		27.96*		07.73*
27		67.14		24.12*		04.21
28		65.26*		20.51*		00.72
29		63.29		16.89*		
30		61.34		13.12		93.80
31		59.39		09.40		90.42*
32		57.31		05.75*		86.81
33		55.27		01.96		83.32
34		53.18		898.18		79.74
35		51.04*		94.32*		76.17
36		48.77		90.45*		72.54
37		46.52*		86.64*		68.87
38		44.15*		82.66*		65.15
39		41.74		78.61		61.40*
40		39.22*		74.55*		57.58*
41		36.71*		70.33		53.68
42		34.11*		66.07*		49.77
43		31.45*		61.82*		45.73
44		28.66*		57.46*		41.67
45		25.83		53.10*		37.55
46		23.00*		48.67*		33.38
47		20.00		43.96		29.15
48		16.89*		39.35		24.79
49		13.73		34.75*	Na-line	20.42
50		10.48*		29.91*		196.48*
51		07.13		24.99		15.93
52		03.69		19.97		11.38*
53		00.09		14.89		06.74*
54		896.34*		09.71		02.02
55		92.59		04.45*		097.21
56		88.55		798.96*		87.8*
57		84.21		93.45		85.0*
58		79.46*		87.70		81.8*
59		73.89*		81.64		78.5*

Table 5 (cont.)

2,0		2,1		2,3	
<i>R (J)</i>	<i>P (J)</i>	<i>R (J)</i>	<i>P (J)</i>	<i>R (J)</i>	<i>P (J)</i>
12866.88	12775.18	12156.90*	12064.99	10765.2	10673.7
57.71	67.82	47.99	58.11	57.3	67.1*
12878.95*	59.23	12170.69	49.82		59.8
69.85*	49.31	61.17*	39.41		50.3*
63.09	12767.75*	54.64	12060.56		
57.46*	56.88*	49.38*	48.93		
52.17	48.52	44.56	40.96		
46.85	41.23	39.71	34.04*		
41.13*		34.43	27.58*		
		28.06	21.03		
		18.81	14.01*		
		26.74	05.99		
		20.15	11995.10	011.25	
		13.97		01.31	
		07.23		11993.12*	
		099.28		85.21	
		121.23*		76.82	
		11.38*		67.21*	
		03.53	87.49	55.38	
		096.76*	75.99		
		90.78	66.48		
		85.07	58.14		
		79.51	50.46		
		73.99	43.06		
		68.54*	35.85		
		63.01	28.70*		
		57.46	21.58		
		51.84			
		46.09			
		40.15			
		34.04*			
		27.58*			
		20.75			
		13.01			
		03.83			
		11992.14	052.16		
		77.33	39.41		
			29.59		
			21.37		
			14.01		
			06.90		
			00.00		
		11933.12			
			86.26		
			79.31		
			72.23		
			65.01*		
			57.37*		
			49.31		
			40.49		
			30.26		
			17.68		

Table 6
Wave-numbers for the 3,0, 3,1 and 3,2 bands

<i>J</i>	<i>R</i> (<i>J</i>)	3,0	<i>P</i> (<i>J</i>)	<i>R</i> (<i>J</i>)	3,1	<i>P</i> (<i>J</i>)	<i>R</i> (<i>J</i>)	3,2	<i>P</i> (<i>J</i>)
11				12957.10*		12938.34			
12				57.00*		36.71*			
13				56.93		35.13*			
14				56.71		33.28			
15				56.39		31.45*			
16				55.98		29.53			12217.37
17				55.54					15.63
18	13676.29			54.98		25.36			13.60*
19	75.50			54.35		23.00			11.46
20	74.70		13641.92*	53.65		20.70		12242.25*	09.29*
21	73.75		39.27	52.84		18.46		41.34	07.09
22	72.75		36.55*	52.02		15.96		40.59*	04.78
23	71.59		34.05*	51.04*		13.42*		39.92*	02.30*
24	70.40		31.21	50.06		10.78*		39.37*	199.98
25	69.19		28.26*	48.98		08.13		38.41	97.58*
26	67.89		25.40*	47.88*		05.34		37.15	94.83
27	66.54		22.28	46.52*		02.50*		36.29	92.22*
28	64.99		19.16	45.23		899.54		35.18*	89.49
29	63.42		16.06	43.85*		96.53		33.93	86.81*
30	61.64		12.80	42.39*		93.53*		32.76*	83.93*
31	59.85		09.58*	40.77*		90.45*		31.27	80.92*
32	57.88		06.04	39.07*		87.17*		30.01*	77.96*
33	55.85		02.55	37.15		83.80		28.08	74.75
34	53.37*		598.62*	34.87		80.40*		25.96*	71.54*
35	50.43*		95.00	31.45*		76.78		22.87*	68.18*
36			90.69		12933.28*	72.69*		18.36*	64.26*
37		13641.92*	86.02		30.90*	67.68			

42	35.81*	919.49	51.52	10.76*	44.57*
43	33.01*	16.89*	47.12		40.88*
44	30.10*	59.13*			
45	27.14	11.58	843.42	210.35	137.24
46	23.87	08.69	39.12	08.17*	33.38*
47	20.54*	05.57	34.75*	05.74	29.15*
48	16.37*	910.78	30.34	03.21*	25.11
49		03.39	25.79*	00.31	20.88*
		895.47	20.89	196.85	16.31
				91.50*	
50		898.98*	15.35*	194.83*	118.81*
51		96.22	07.38	91.50*	11.10
52		91.60	09.25	88.02*	04.08
53		87.87*	03.72	84.63*	05.63*
54		83.80*	798.34	80.92*	00.57
55		79.11*	92.89	76.76*	095.53
56	896.34*	73.36	87.12	71.29	90.41*
57	87.17*	66.07*	80.72		85.07*
58	80.15		73.26		79.07
59	74.55*		85.37		094.90
					84.45
60	69.85*		76.59*	69.35*	76.11
61	65.43*		69.39	65.52*	69.50
62	61.20		62.96	61.40*	63.29
63	57.06		56.88*	57.87	57.65
64	52.90		50.96	53.95*	52.19*
65	48.67*		45.10	50.40	46.67*
66	44.51		39.22	46.60	41.36
67	40.43			42.83	35.97
68	35.94			38.98	30.50
69	31.57			35.02*	25.04
70	27.14*				
71	22.64			31.14	19.58
72	18.22			27.14	14.01*
73	13.60			23.00	08.39
74	08.89			18.81*	02.72
75	04.15			14.64	11996.94
76				10.07	91.11
77					86.21*
					79.02

Table 7
Wave-numbers for the 4,1 and 4,2 bands

<i>J</i>	4,1		4,2	
	<i>R</i> (<i>J</i>)	<i>P</i> (<i>J</i>)	<i>R</i> (<i>J</i>)	<i>P</i> (<i>J</i>)
12			12947.88*	
13	13660.32		47.88*	
14	59.85*		47.60	12924.32
15	59.31	13634.81*	47.25	22.51
16	58.87	32.60	46.96	20.51*
17	58.34	30.51*	46.52*	18.46*
18	57.76	28.26*	46.11	16.51
19	57.05	25.91*	45.53	14.33*
20	56.29	23.54*	44.87	12.17
21	55.37	21.03*	44.15*	09.77
22	54.50	18.51*	43.43*	07.44
23	53.37*	16.06	42.39*	04.95
24	52.32	13.17	41.50	02.50*
25	51.02	10.46*	40.39	899.80
26	49.34*	07.51*	38.91* 12943.43*	97.09*
27	Ca-line 13650.43*	04.65*	36.18* 40.09	94.32*
28	41.92*	01.14*	31.85 38.01	91.08 12895.47*
29	Ca-line	596.61* 13600.47*	36.50*	86.64* 90.45*
30	44.77	90.11 596.44*	35.13*	80.40* 86.64*
31	43.14*	92.87	33.61	83.42*
32	41.42*	89.57*	32.14	80.40*
33	39.60*	86.20	30.55*	77.14
34	37.75*	82.82*	28.94	73.89*
35	35.81*	79.21*		70.59
36	33.80*	75.59*		67.22
37	31.72*	71.92	23.65	63.79
38	29.55	68.15	21.75	60.31*
39	27.31*	64.35	19.79	56.76*
40	25.02*	60.47*	17.78	53.10*
41	22.67*	56.52*	15.68	49.45
42	20.19	52.50	13.42*	45.69
43	17.61*	48.37	11.21	41.87*
44	15.02	44.17*	08.88	37.99
45	12.32*	39.93*	06.51	34.06*
46	09.58*	35.54	04.04	29.91*
47	06.79		01.55	25.79*
48	03.89		898.98*	21.78*
49	00.94	22.07	96.34*	17.58*
50	597.90*	17.53	93.53*	13.29*
51	94.67	12.78	90.76*	08.89*
52	91.47	08.08*	87.87*	04.45*
53	88.11*	03.16	85.00	799.97
54	84.86	498.25	82.04	95.41
55	81.42	93.24	78.97*	90.80
56	77.87	88.19*	75.85	86.10
57	74.27	83.03	72.69*	81.33
58	70.61*	77.78	69.34	76.59*
59	66.93	72.53	66.07*	71.62
60	63.18*	67.14	62.58	66.77*
61	59.13*	61.69	59.10	61.56
62	55.17	56.18*	55.54*	56.56
63	51.10*	50.62	51.84*	51.37
64	46.49	44.91	47.73	46.14
65	40.11	39.09	41.87*	40.80
66		32.89		
67		24.71		

Table 8

Wave-numbers for the 5,2, 5,3 and 6,3 bands

5,2		5,3		6,3	
<i>R</i> (<i>J</i>)	<i>P</i> (<i>J</i>)	<i>R</i> (<i>J</i>)	<i>P</i> (<i>J</i>)	<i>R</i> (<i>J</i>)	<i>P</i> (<i>J</i>)
641.42*		12940.09*		13637.75	
40.62		39.22*		37.11	
39.60*	13600.47*	38.34*		36.12*	13598.62*
38.47	597.90*	37.43	12897.09	35.13	96.44*
37.37	95.22	36.50*	94.32	34.05	93.79*
36.12*	92.41	35.34	91.60*	33.01*	91.02*
34.81*	89.57*	34.11*	89.04	31.62*	88.11*
33.47	86.58	33.28*	86.21	30.10*	85.65*
				28.26*	82.30
32.05	83.53	31.85*	83.42*	25.91*	79.21*
30.51*	80.38	30.55*	80.40*	22.67* 13628.26*	75.59*
29.04*	77.19*	29.18	77.49	25.02*	71.55
27.31*	74.05*	27.96*	74.55*	22.67*	66.63 13572.28*
25.40*	70.61		71.43*	20.54*	67.32*
23.54*	67.32*	24.57	68.20	18.51*	63.18*
21.68	63.76	23.00*	64.93	16.37*	59.38*
19.67	60.23	21.10	61.82*	14.31*	55.56
17.61*	56.52*	19.29	58.28	12.32*	51.69
15.24	52.80	17.29	54.76	10.08	47.89
12.32* 13621.03*	48.92		51.23	07.89	44.17*
08.18 14.31*	44.93	12916.89*	47.43	05.67	40.29*
10.46*	40.29 13548.92*	13.42*		03.29	36.45
07.51*	34.44 40.66	10.48*	12851.84*	01.14*	
04.79	35.12*	08.13*	38.50	598.62*	
02.08		05.75*	34.06*	96.21*	24.50
599.36	25.87	03.39*	29.91*	93.79*	20.34
96.61	21.42	00.95	25.79*	91.02*	16.22
93.79*	17.13	898.50	21.78*	88.39	12.00
91.02*	12.66	95.97	17.58*	85.65*	07.72
88.11*	08.08*	93.53*	13.29*	82.82*	03.31
85.10	03.54	90.76*	09.25*	80.03	498.94*
82.00	498.94*	87.87*	05.25	77.19*	94.42
78.87	94.28	85.26	00.63	74.05*	89.95
75.59*	89.50	82.66*	796.22*	71.08	85.32
72.28*	84.61	79.46*	91.80	67.94	80.64
68.92	79.75	76.49	87.12*	64.74*	75.88
65.17	74.75	73.09	82.66	61.41	71.11
60.47	69.62		77.91	58.10	66.20
53.60	64.18		72.72	54.64*	61.27
	57.55		66.77	51.10*	56.18*
	49.29			47.47	51.02
				43.67	45.91
				39.93*	40.82
				36.13	35.68
					30.55
					25.18
					19.83

tions at $J \sim 53$. It will be seen that for many of the perturbations, the two (three) companion lines have been found for several J -values. The columns are not altered at the perturbations in $v' = 0$ at $J \sim 95.5$, in $v' = 1$ at $J \sim 81$ and in $v' = 2$ at $J \sim 64.5$. It is difficult here to state where the perturbation culminates, as another stronger perturbation always occurs just at the lower J -values.

Calcium has four isotopes, but of these ^{40}Ca is much the most abundant (96.8 %); the next most common being ^{44}Ca (2.3 %). We have made no effort to measure lines other than those attributed to ^{40}Ca .

§ 4. Determination of rotational constants

The rotational constants for the lower unperturbed v'' -levels have been determined with the weighted centre-of-gravity method (see BARROW, LAGERQVIST and LIND, 1950). The values are given in Table 9.

Other methods have been used to calculate the rotational constants for the upper perturbed v' -levels. The method introduced by GERÖ (1935) for detecting perturbations in the upper state have been used. The following expression is formed

$$\frac{R(J-2) - R(J-1) + P(J) - P(J+1)}{4J} = B'' - B' + 6D'' - 2J^2(D'' - D').$$

If the left hand side of this expression is plotted against J^2 , ΔB is obtained as the intercept at $J = 0$. ΔD is obtained from the slope. The unperturbed regions, in which the points lie on an almost horizontal line, were used. As B'' and D'' had already been determined, B' and D' could be calculated.

The D' -values thus obtained were compared with those obtained from $\Delta^2 F'(J)/(J + \frac{1}{2})$ plotted against $(J + \frac{1}{2})^2$ for certain unperturbed regions of the upper levels. The agreement was good (0.54×10^{-6} in both cases).

The values are given in Table 9.

We estimate the errors in the B'' -values as about ± 0.00005 ; for B'_0 the error is about $\pm 0.0001 \text{ cm}^{-1}$.

As will be seen from Table 9, the B' -values vary somewhat irregularly with v' ; this depends, of course, on the fact that in some of these vibrational levels none of the rotational levels is entirely unperturbed. We would also stress that for such strongly perturbed levels it is meaningless to speak of a fixed B -value, as the B -value varies from one rotational level to the next. Usually the B -value given is that nearest to the "unperturbed" one. In reality every rotational level has a B -value that is a mixture of the B -values of the perturbed and perturbing states.

Table 9

Rotational Constants for the $^1\Sigma$ and $^1\Sigma^*$ -states

v	$B''_{\text{obs.}}$	$B''_{\text{calc.}}$	$D''_{\text{obs.}}$	$D''_{\text{calc.}}$	$B'_{\text{obs.}}$	$B'_{\text{calc.}}$
0	0.4428 ₀	0.4428 ₀	0.65 ₉ · 10 ⁻⁶	0.659	0.4056	0.4056
1	0.4394	0.4394 ₈	0.65 ₃	0.662	0.4030	0.4042
2	0.4362	0.4361 ₃	0.66 ₉	0.665	0.4022	0.4028
3	0.4328	0.4328 ₁	0.67 ₂	0.668	0.4016	0.4014
4					0.4003	0.4000
5					0.3986	0.3985
6					0.3965	0.3971

The calculated values are found from the expressions:

$$B''_v = 0.4444_7 - 0.0033_5(v + \tfrac{1}{2}) + 0.00000_5(v + \tfrac{1}{2})^2$$

$$D''_v = [0.658 + 0.003(v + \tfrac{1}{2})] \times 10^{-6}$$

$$B'_v = 0.4063 - 0.0014_1(v + \tfrac{1}{2}).$$

D' is found to be 0.54×10^{-6} .

The internuclear distances are:

$$r''_e = 1.822 \times 10^{-8} \text{ cm and } r'_e = 1.906 \times 10^{-8} \text{ cm.}$$

With the values for ω''_e and ω'_e in § 7, we obtain, from KRATZER's relation ($D = 4B^3/\omega^2$), $D'' = 0.66 \times 10^{-6}$, $D' = 0.52 \times 10^{-6}$, which agree satisfactorially with the experimental values.

§ 5. Some relations between band-constants at perturbations between n electronic states

At a perturbation between two electronic states companion lines are often found in the spectrum. In such cases it is possible to calculate the band-constants of the perturbing state. The theoretical treatment for singlet-singlet interactions is given by KOVÁCS (1937 a). On the other hand no example is found — so far as we know — where companion lines are found at interactions between three electronic states. In the 0,0 band (8652) of the infra-red CaO system the upper level is perturbed by two electronic states at about $J = 53$. For seven J -values (51, . . . , 57) of the upper state three P and three R -lines have been found. It is therefore desirable to deduce expressions for the relations between the B and C -values of three interacting states. As there is a little chance of finding perturbations between more than three electronic states, we shall treat here the general case between n states. Our intention is only to give expressions for the B and C -values, not to investigate the course of the interacting energy levels, which requires a study of the secular equation of the n^{th} degree. KOVÁCS and SINGER (1942) have published a paper on this mutual reactions between three spectral terms, but they have not given any expressions for the determination of B and C -values.

Fig. 4 shows the interaction between n electronic states with energies $W_1, \dots W_n$. We assume that a transition $W_1 \rightarrow W_0$ is studied. The upper level

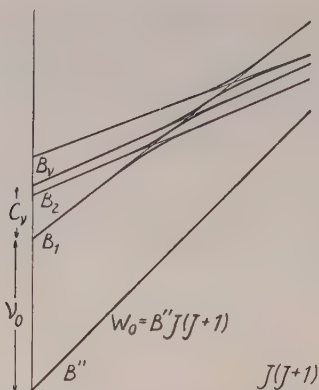


Fig. 4. Energy levels for a singlet-singlet interaction of n -states in the upper level.

W_1 is thus perturbed. The distance between W_1 and W_0 at $J = 0$ is called ν_0 . The distance between any of the perturbing states and W_1 at $J = 0$ is called $C_1, C_2, \dots, C_n$. Thus $C_1 = 0$. The B -values of the interacting terms are called $B_1, B_2, \dots, B_n$. (The suffixes do not, of course, allude to vibrational quantum numbers). In the perturbed region the energy of a term W_v is written

$$W_v = \nu_0 + C_v + \varepsilon_v + B_v J(J+1), \quad (1)$$

where ε_v is the magnitude of the deviation. The lower state is given by

$$W_0 = B'' J(J+1).$$

The mean value of all terms W_v , $\frac{\sum W_v}{n}$, is unperturbed (see Kovács, 1937 b) and taking this into consideration, $\sum \varepsilon_v = 0$, we have

$$\frac{\sum W_v}{n} = \nu_0 + \frac{\sum C_v}{n} + J(J+1) \frac{\sum B_v}{n}. \quad (2)$$

If R and P -branches only are present, all states are Σ -states, and $\frac{\sum W_v}{n}$ can be expressed with the R or the P -lines or if both branches are investigated with the mean of terms from the R and P -branches. Thus we have

$$\begin{aligned} \frac{\sum W_v}{n} &= \frac{1}{2n} \sum [R_v(J-1) + P_v(J+1)] + \frac{1}{2} [B''(J+1)(J+2) + B''(J-1)J] = \\ &= \frac{1}{2n} \sum [R_v(J-1) + P_v(J+1)] + B''(J^2 + J + 1). \end{aligned} \quad (3)$$

$\frac{\sum W_v}{n}$ is hence given by both Equ. (2) and (3). Putting (2) equal to (3) for J and $(J-1)$, we obtain two equations, from which $\frac{\sum B_v}{n}$ and $\frac{\sum C_v}{n}$ can be solved.

Making the abbreviation

$$T_v(J) = R_v(J-1) - R_v(J-2) + P_v(J+1) - P_v(J) \quad (4)$$

we get,

$$\frac{\Sigma B_v}{n} - B'' = \frac{1}{n4J} \Sigma T_v(J), \quad (5)$$

$$\begin{aligned} \frac{\Sigma C_v}{n} = & -v_0 + B'' + \frac{1}{4n} \{ \Sigma [R_v(J-2) + P_v(J)](J+1) - \\ & - \Sigma [R_v(J-1) + P_v(J+1)](J-1) \}. \end{aligned} \quad (6)$$

From these equations, (5) and (6), ΣB_v and ΣC_v can be solved. In this expression $C_1 = 0$ of course.

Putting $n = 2$, we obtain the equations derived by KOVÁCS (1937 a).

Taking into consideration the effect of the D -values, small corrections must be added to the energies ($W = BJ(J+1) - DJ^2(J+1)^2$). The result is

$$\frac{\Sigma B_v}{n} - B'' = \frac{1}{n4J} \Sigma T_v(J) + 2J^2 \frac{\Sigma D_v}{n} - 2D''(J^2 + 3), \quad (7)$$

$$\begin{aligned} \frac{\Sigma C_v}{n} = & -v_0 + B'' + \frac{1}{4n} \{ \Sigma [R_v(J-2) + P_v(J)](J+1) - \\ & - \Sigma [R_v(J-1) + P_v(J+1)](J-1) \} - 2J^2(J^2-1) \frac{\Sigma D_v}{n} + 2(J^2+1)(J^2-2)D''. \end{aligned} \quad (8)$$

It is, of course, possible to solve ΣD_v in the same way as ΣB_v and ΣC_v if we write the expressions for $\frac{\Sigma W_v}{n}$ for $(J+1)$, J and $(J-1)$ in (2) and (3). We then get three equations for obtaining ΣB_v , ΣC_v and ΣD_v . They are of course of such ungainliness that they are of no practical value. Usually the effect of the D -values is insignificant. If their effect is to be estimated the simplest way is to calculate rough D -values from KRATZER's relation and use Equ. (7) and (8).

If the R -branch only is known, we obtain Equ. (9) and (10) instead of (5) and (6)

$$\frac{\Sigma B_v}{n} = B'' \frac{(J-1)}{J} + \frac{1}{n2J} \Sigma [R_v(J-1) - R_v(J-2)], \quad (9)$$

$$\frac{\Sigma C_v}{n} = -v_0 - B''(J-1) + \frac{1}{2n} \{ \Sigma [R_v(J-2)](J+1) - \Sigma [R_v(J-1)](J-1) \}. \quad (10)$$

If only the P -branch is known, we can use Equ. (11) and (12)

$$\frac{\Sigma B_v}{n} = B'' \frac{(J+1)}{J} + \frac{1}{n2J} \Sigma [P_v(J+1) - P_v(J)], \quad (11)$$

$$\frac{\Sigma C_v}{n} = -v_0 - B''(J+1) + \frac{1}{2n} \{ \Sigma [P_v(J)](J+1) - \Sigma [P_v(J+1)](J-1) \}. \quad (12)$$

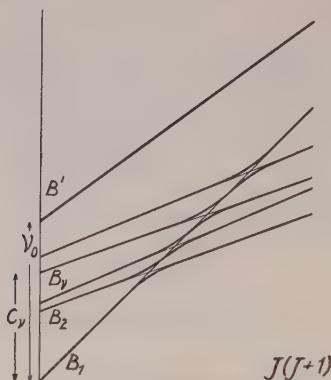


Fig. 5. Energy levels for a singlet-singlet interaction of n -states in the lower level.

If we have a Π — Σ transition, and a perturbation in the upper level is studied in the Q -branch, Equ. (13) and (14) are valid, if the energies of the Π -states are written in the form $W = B J(J+1)$ instead of the correct form $W = B[J(J+1) - 1]$ (Equ. (13) is valid in both cases).

$$\frac{\Sigma B_v}{n} - B'' = \frac{1}{n 2 J} \Sigma [Q_v(J) - Q_v(J-1)], \quad (13)$$

$$\frac{\Sigma C_v}{n} = -v_0 + \frac{1}{2n} \{ \Sigma [Q_v(J-1)](J+1) - \Sigma [Q_v(J)](J-1) \}. \quad (14)$$

In all these equations (5)—(14) it is assumed that the upper level is perturbed. If the perturbation takes place in the lower state, we obtain Equ. (15) and (16), which correspond to (5) and (6). The lower perturbed state is given the suffix 1. The notations can be seen in Fig. 5.

The equations are

$$\frac{\Sigma B_v}{n} = B' - \frac{1}{n 4 J} \{ \Sigma [R_v(J) - R_v(J-1) + P_v(J) - P_v(J-1)] \}, \quad (15)$$

$$\begin{aligned} \frac{\Sigma C_v}{n} = v_0 + B' - \frac{1}{4n} \{ \Sigma [R_v(J-1) + P_v(J-1)](J+1) - \\ - \Sigma [R_v(J) + P_v(J)](J-1) \}. \end{aligned} \quad (16)$$

§ 6. Perturbations

a) Treatment of the perturbations

We have found in all more than thirty perturbations in the upper state levels from $v' = 0$ to $v' = 6$. From their appearance we can conclude that all perturbing levels have B -values lower than B' . In several of the perturbations companion lines are found (see Tables 3—8). Figs. 2 and 3 show the appearance

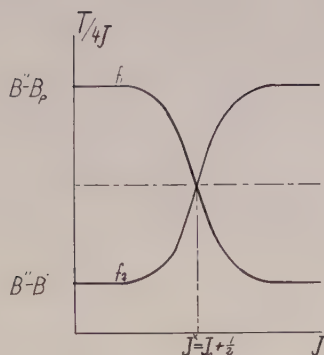


Fig. 6. The variation of $T/4J$ for a singlet-singlet interaction.

of the 0,0, 1,0 and 2,1 bands. The spectrograms reproduced show clearly how strong some of the perturbations are, and it is easy to see that they make the analyses difficult. In the 0,0 band two perturbing electronic states interact with the Σ^* -state at about the same J -values. Every rotational Σ^* -level is here split up into three levels. This perturbation will be discussed further in § 6 b.

The perturbations have been studied by GERÖ's method (1935). We have

$$\frac{T}{4J} = \frac{R(J-2) - R(J-1) + P(J) - P(J+1)}{4J} = B'' - B' + 6D'' + 2(D' - D'')J^2.$$

$T/4J$ is plotted against J , for unperturbed regions an almost horizontal line is obtained. At a perturbation, two $T/4J$ curves are obtained, one for each energy term. (See Fig. 6.) The theoretical expressions f_1 and f_2 for the two branches of $T/4J$ have been given by KOVÁCS (1937 a). They contain, of course, the perturbing matrix elements. The point of intersection of f_1 and f_2 , which is equal to $\frac{1}{2}(f_1 + f_2)$, gives the perturbing B -value (Equ. 5). The J -value at the intersection, J^* , is approximately related to the J -value at which the perturbation culminates, J_0 , by the simple equation

$$J_0 \sim J^* - \frac{1}{2}. \quad (17)$$

The C -values can be determined from Equ. (6). They can also be calculated as

$$C = (B' - B_p) J_0 (J_0 + 1). \quad (18)$$

The plots of $T/4J$ against J for all the bands, except the weak 3,0 band, are given in Figs. 7, 8 and 9. The error in $T/4J$ -increases of course, as J decreases, so that the scatter of the points becomes rather considerable at low J -values.

Some data obtained on the perturbations is summarized in Table 10 and in Fig. 10. The positions of the states and of the perturbations are indicated in a plot against $J(J+1)$. In the diagram, circles indicate the positions where the perturbations culminate. Table 10 contains the B -values of the perturbing

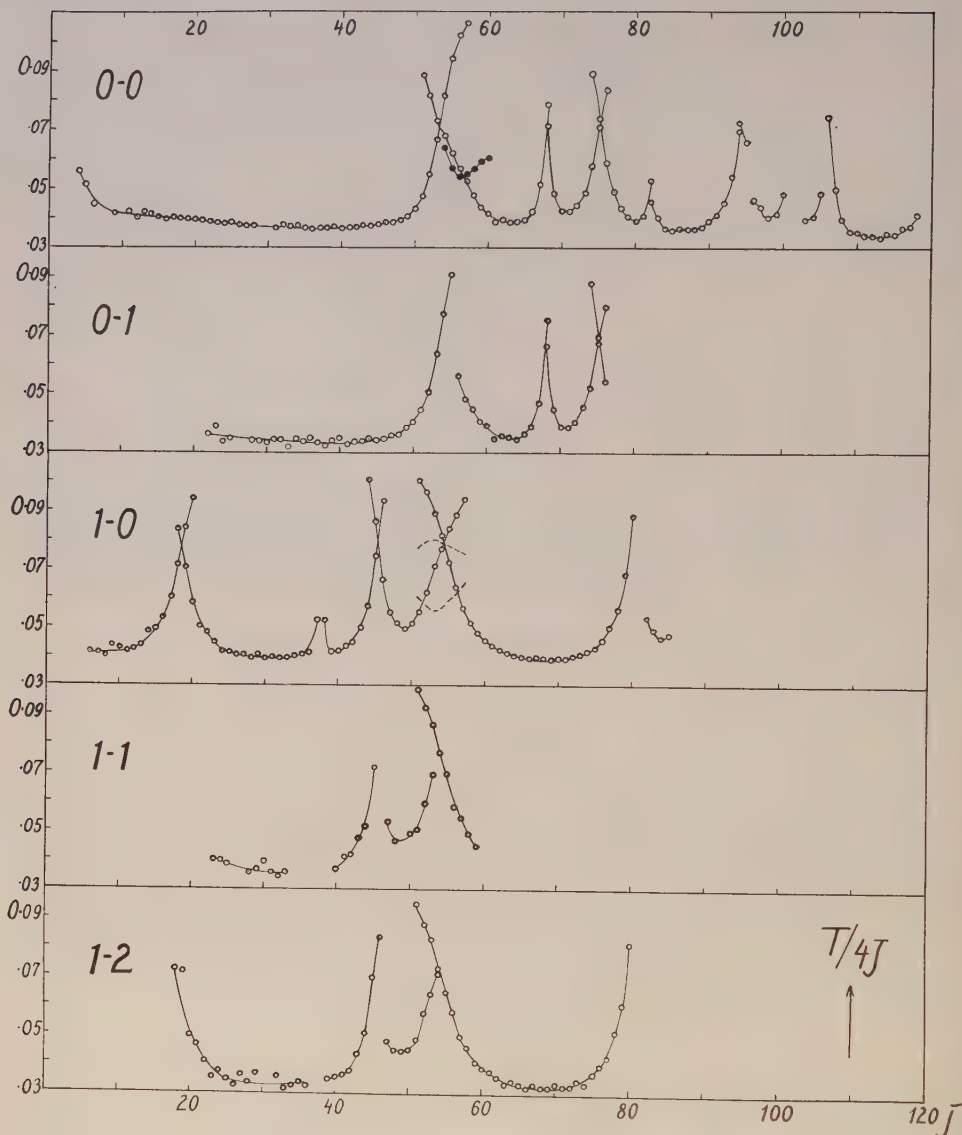


Fig. 7. $T/4J = [R(J-2) - R(J-1) + P(J) - P(J+1)]/4J$ plotted against J for the 0,0, 0,1, 1,0, 1,1 and 1,2 bands. In the 0,0 band at $J \sim 53$ three states interact. The plots of $T/4J$ for one of these levels are indicated by filled circles. In the 1,0 band at $J \sim 53$ two curves are drawn with broken lines. The upper curve represents the means of $T/4J$, the lower one the $T/4J$ curve for the undetected third interacting state.

states calculated from Equ. (5). Most of the B -values are of the magnitude 0.33, some of them about 0.38. The estimated error is given for every B -value determined. The error depends not only on the number of determinations, which is given in brackets, it depends also on the quality of the lines used (whether

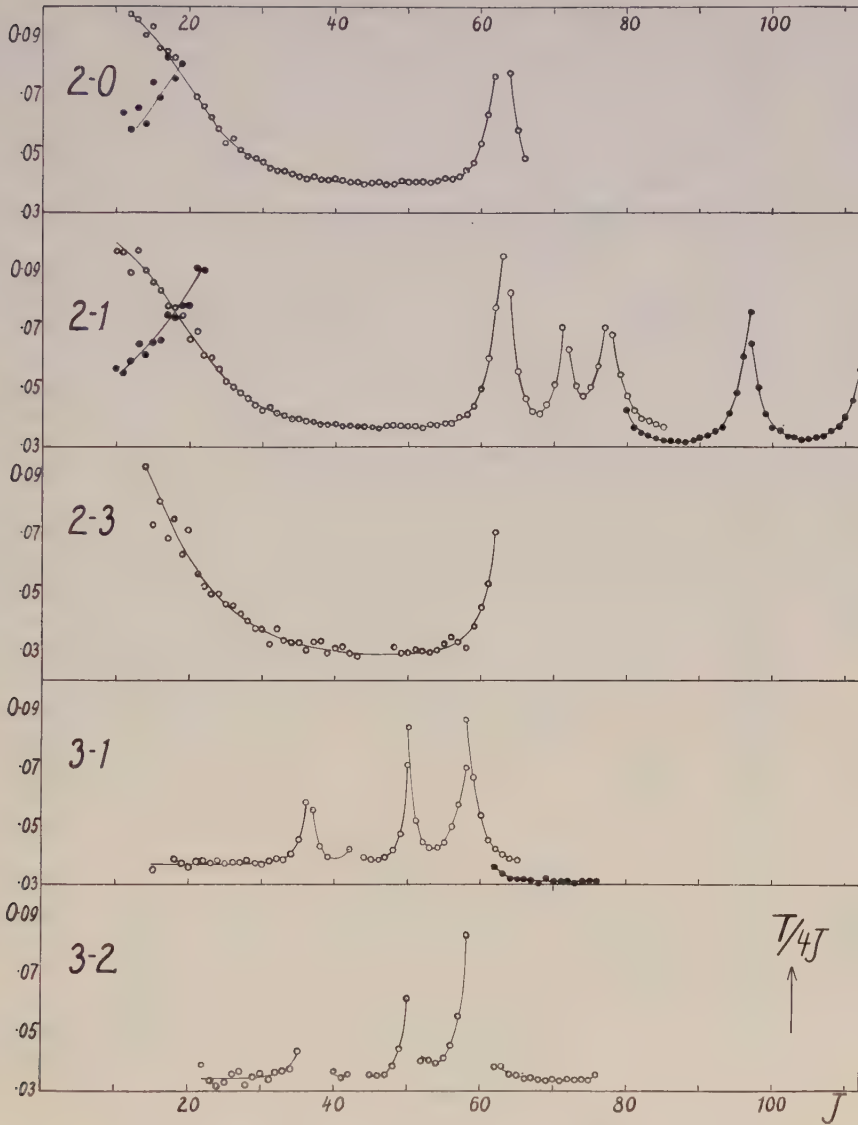


Fig. 8. $T/4J$ plotted against J for the 2,0, 2,1, 2,3, 3,1 and 3,2 bands. In the 2,0 and 2,1 bands for the perturbation at $J \sim 18$, the plots for one of the interacting levels are indicated by filled circles. At the ends of the 2,1 and 3,1 bands, filled circles indicate plots of $\frac{1}{2J} [R(J-2) - R(J-1)]$.

they are overlapped, well defined, etc.). The perturbations can be explained by assuming the existence of six perturbing electronic states or substates, four of them are called X , Y , Z and Q and have B -values of about 0.33, the other two A and B having B -values of about 0.38. It is, however, difficult to decide which state perturbs the level $v' = 2$ at $J \sim 113$.

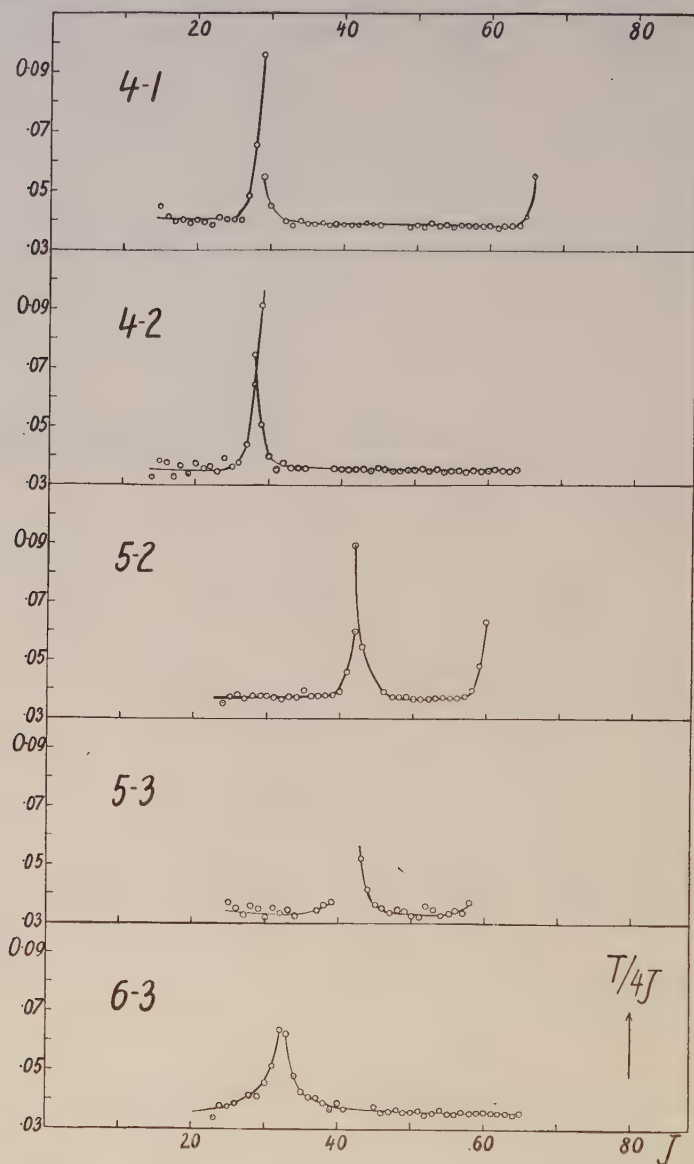


Fig. 9. $T/4J$ plotted against J for the 4,1, 4,2, 5,2, 5,3 and 6,3 bands.

In the 2,1 and 3,1 bands only the R -lines are traced above $J = 85$ and $J = 65$, respectively. In Fig. 7 and 8, $\frac{1}{2J}[R(J-2) - R(J-1)]$ are plotted against J . The perturbing B -value at $J^* = 96.7$ in $v' = 2$ is calculated from Equ. 9. As $v' = 0$ is also perturbed by all the six states A , B , X , Y , Z and Q , it is impossible to decide the absolute vibrational quantum numbers for these states.

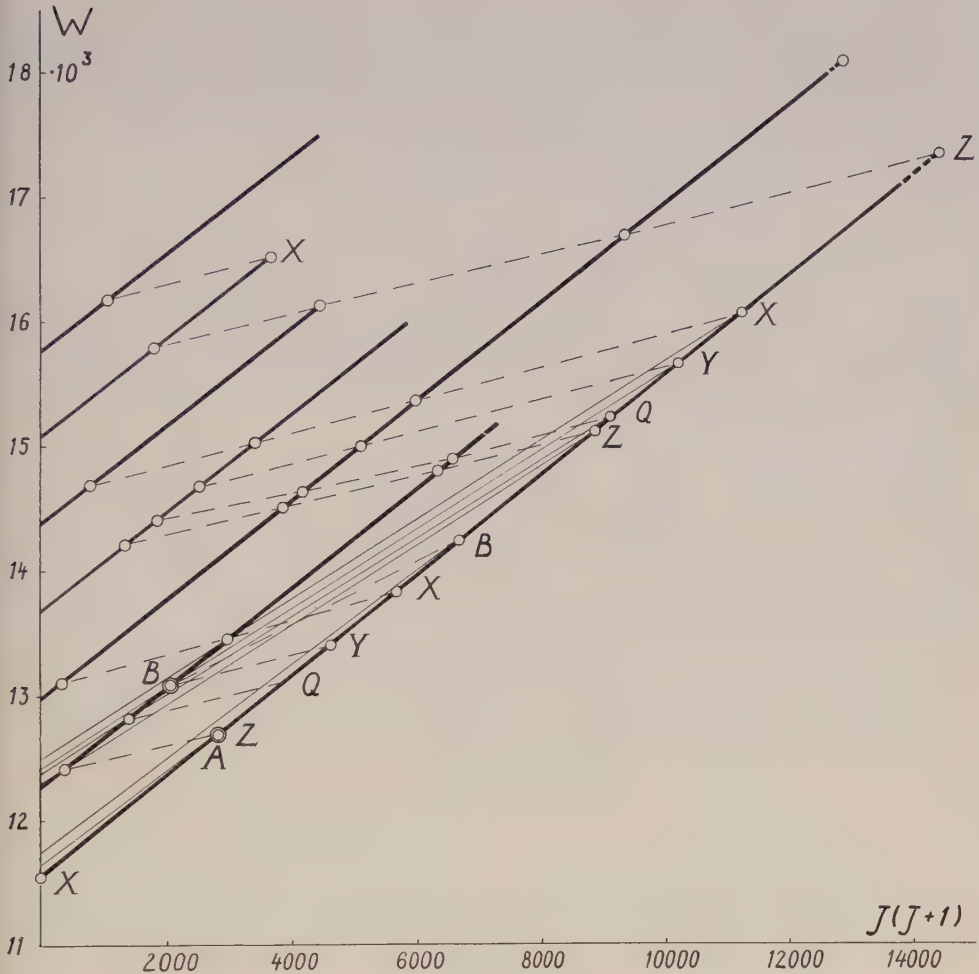


Fig. 10. Perturbations in CaO-term values plotted against $J(J+1)$. Σ^* : thick lines for the parts analysed, broken lines for the extrapolated regions. Perturbing states: thin lines. For the sake of surveyability only the lowest perturbing levels are drawn. Double circles indicate double perturbations.

The lowest vibrational levels found are indicated by a , b , x , y , z and q . A Q -perturbation ought to lie at about $J = 62$ in $v' = 0$. No perturbation is found here. All the Q -perturbations are, however, very weak, and it is therefore uncertain whether the lowest q -level found is the one with $v = 0$. We have indicated it here by q .

The perturbation at $J \sim 54$ in $v' = 1$ gives different values for the means of $\frac{1}{2}(f_1 + f_2) = \frac{1}{2} \left(\frac{T_1}{4J} + \frac{T_2}{4J} \right)$ indicating a double perturbation. It is most probable that both X and B interact at this point.

No B -values have been calculated for the Q -state. Its perturbations with Σ^* show, however, that B_q is of the same order as B_x , B_y and B_z . In the higher v' -levels Q and Y -perturbations are lacking. This must depend on the small matrix elements. The matrix elements of the X -perturbations are also much smaller here than in the lower v' -levels.

The B -values can be fitted into the equations:

$$B_{x+v} = 0.32_9 - 0.001_4 v$$

$$B_{y+v} = 0.32_8 - 0.001_6 v$$

$$B_{z+v} = 0.33_0 - 0.001_5 v.$$

They can be written approximately as: $B_v = 0.33_0 - 0.00_{15} v$. B_b is found to be 0.38_1 , and $(B_a + B_z) = 0.7103$. As $B_z = 0.33_0$ we obtain $B_a = 0.38_0$.

Table 10
Summary of the perturbations

$v'(\Sigma^*)$	J^*	B_p (number of determinations in brackets)	Perturbing state	vp
0	~ 0	The sum 0.7103 (4) $\pm$ 0.0005	X	x
0	~ 53		Z	z
0	~ 53		A	a
0	67.9		Y	y
0	75.2		X	$x+1$
0	81.7	0.381 (1) $\pm$ 0.005	B	b
0	94.1	0.337 (1) $\pm$ 0.008	Z	$z+1$
0	~ 95.5	—	Q	q
0	~ 101	—	Y	$y+1$
0	~ 106	—	X	$x+1$
0	~ 120	—	Z	$z+2$
1	19.5	0.328 (3) $\pm$ 0.002	Z	$z+1$
1	~ 37.5	—	Q	q
1	45.3	0.323 (3) $\pm$ 0.002	Y	$y+1$
1	54.2	0.327 (14) $\pm$ 0.002	$X(B)$	$x+2$
		two perturbations		($b+1$)
1	~ 79.5	—	Z	$z+2$
1	~ 81	—	Q	$q+1$
2	18.5	0.3250 (15) $\pm$ 0.0005	X	$x+3$
2	~ 62	—	Z	$z+3$
2	~ 64.5	—	Q	$q+2$
2	~ 71.3	—	Y	$y+3$
2	~ 77.3	—	X	$x+4$
2	96.7	0.325 (1) $\pm$ 0.005	Z	$z+4$
2	~ 113.5	—	$?$	$?$
3	~ 36.4	—	Z	$z+4$
3	~ 43	—	Q	$q+3$
3	50.2	0.322 (1) $\pm$ 0.005	Y	$y+4$
3	58.4	0.320 (1) $\pm$ 0.005	X	$x+5$
4	28.2	0.329 (3) $\pm$ 0.004	X	$x+6$
4	~ 66.5	—	Z	$z+6$
5	42.3	0.325 (1) $\pm$ 0.005	Z	$z+7$
5	~ 60.5	—	X	$x+8$
6	~ 32.5	—	X	$x+9$

The C -values are determined from Equ. (6), (12) and (18). The term values at $J = 0$, $(T_{v'} + C)$ are given in Table 11. The following vibrational constants have been derived:

$$\begin{array}{lll} \omega_x = 500 & \omega_y = 506 & \omega_z = 508 \\ x\omega_x = 0.9 & x\omega_y = 1.7 & x\omega_z = 1.6. \end{array}$$

Table 11

Term values of the perturbing states at $J = 0$

v_x	T_{x+v}	v_y	T_{y+v}	v_z	T_{z+v}	v_p	T_a or T_b
$x+1$	11989	y	11907	z	11763	b	11748
$x+2$	12494	$y+1$	12422	$z+1$	12286	$b+1$	12329
$x+3$	12993	$y+3$	13370	$z+2$	12744	a	11650
$x+4$	13437	$y+4$	13875	$z+3$	13264		
$x+5$	13953			$z+4$	13770		
$x+6$	14438			$z+6$	14724		
$x+7$	15367			$z+7$	15213		
$x+8$	15505						

They are approximately of the order $\omega = 500$, $x\omega = 1.5$.

The states A and B give birth to only three perturbations altogether. The value $T_a = C_a + 11549$ can be calculated from Equ. (6), in which in this case $n = 3$. We get

$$C_a + C_z = 311,$$

But $C_z = 208$ (C_z obtained as the mean of all the T_{z+v} -values calculated with $\omega_z = 508$ and $x\omega_z = 1.6$). This gives $C_a = 101$. The T_a and T_b -values are given in Table 11. ω_B is of the order 600. It is easy to investigate that if $\omega_A = \omega_B \sim 600$ the terms of A and B do not cut the Σ^* -levels studied at any other places than those at which the three perturbations have been found.

b) Perturbations between three interacting states

At about $J \sim 53$ three R - and three P -lines have been found (see Fig. 2). Plotting $T/4J$ against J we obtain three curves in the perturbed region (Fig. 7). This very curious perturbation depends on an interaction of Σ^* with two electronic states. Every rotational level of Σ^* is split up into three levels. As far as we know, this is the first published example of such a perturbation.

Owing to the courses of the three interacting "unperturbed" levels, the real energy levels and the $T/4J$ -plots become different. In Fig. 11 we have drawn some examples of such curves (further examples can be drawn). It seems to us that Fig. 11 c is the case corresponding to the perturbation studied.

The sum of the B -values of the interacting states can be calculated from Equ. (5), the sum of the corresponding C -values from Equ. (6). In these equations we have to put $n = 3$. The agreement between the values obtained is

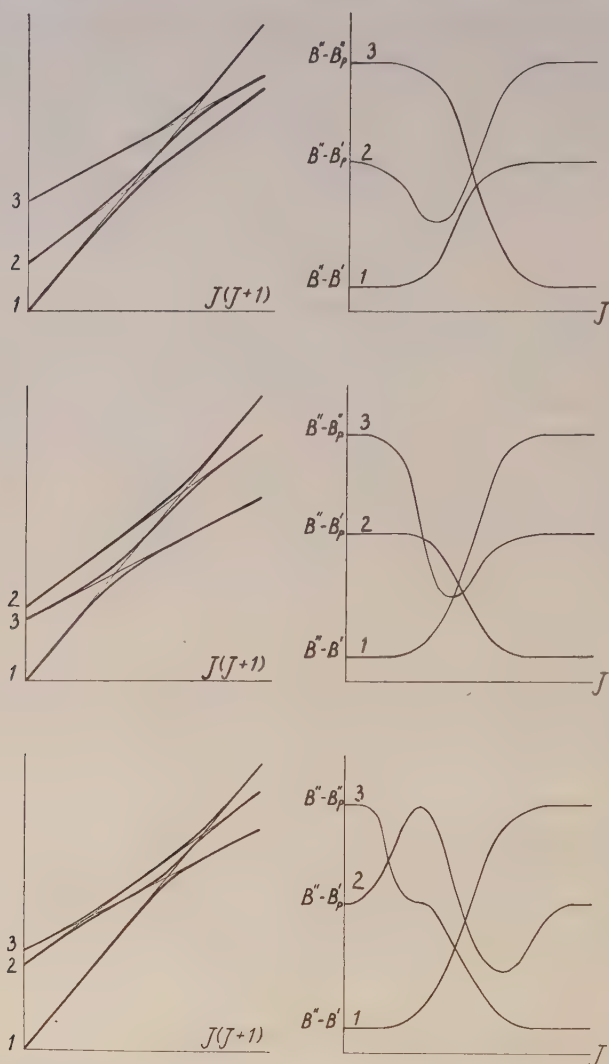


Fig. 11. The three left-hand diagrams represent the courses of the energy levels for three interacting singlet states 1, 2 and 3 with the B -values B' , B'_p and B''_p . B'' is the B -value for a lower state not drawn in the figures. The three right-hand diagrams show the corresponding $T/4J$ -curves. Fig. 11 c corresponds to the perturbation at $J \sim 53$ in the 0,0 band.

very good. Table 12 shows the result. The table gives the sum of the B -values $B'_p + B''_p$ of the perturbing states — B' is 0.4030 — and the sum of the C -values $C'_p + C''_p$ ($C' = 0$).

As we know the magnitude of B and C for one of the perturbing states (Z), 0.33 and 208, the constants for the other can be obtained. Unfortunately we do not know B_z and C_z with any high degree of accuracy.

Table 12

J	$B'_p + B''_p$	$C'_p + C''_p$
54	0.7108	310.97
55	0.7099	311.78
56	0.7100	311.34
57	0.7103	310.35
Mean	0.7103	311.1

We did not obtain a constant value when taking the means of $T_1/4J$ and $T_2/4J$ for determining the B -value (B_{x+3}) at the perturbation at $J \sim 54$ in the level $v' = 1$. In Fig. 7 we have drawn a broken line through the means of curves (concave towards the J -axis). Assuming another perturbing state is present — everything points to B_{b+1} — the $T/4J$ plots for this state ought to give a curve convex towards the J -axis (another broken line is drawn here in Fig. 7). The means of $T/4J$ for the three interacting terms must give a constant value. We have searched for lines in the 1,0 band corresponding to this third level but without success. They must be very weak, otherwise we ought to have found them. In the background there are some weak lines, but it is difficult to form trustworthy series. The analysis is also difficult owing to all the perturbed series in the 1,0 and 2,1 bands. It is very probable that some of the lines are overlapped by strong lines belonging to these branches. Although we have not found lines from this third level we are quite sure that they exist, otherwise the means of $T_1/4J$ and $T_2/4J$ ought to have given a constant value.

c) Nature of the perturbing states

The appearance of the perturbations in CaO reminds one very much of those in SrO (ALMKVIST, LAGERQVIST, 1950) and BaO (BARROW, LAGERQVIST and LIND, 1950). The CaO ${}^1\Sigma - {}^1\Sigma$ system is perturbed by four states with about the same B and ω -values exactly as is the case in BaO and SrO. In the case of CaO the richness of companion lines is not so great as in the case of BaO (for a detailed discussion on the nature of the perturbing states here see KOVÁCS and LAGERQVIST, 1950). In spite of the great number of companion lines in the BaO spectrum, it was impossible to decide with absolute certainty if the perturbing states are singlets or triplets or of both types. Besides the four states with B -values and ω -values of the order 0.33 and 500, the upper CaO state levels are also perturbed by two other states having $B \sim 0.38$ and $\omega \sim 600$. We can therefore not conclude very much regarding the nature of the perturbing six states in CaO. On the contrary it is very probable that the bands further out in the infra-red (above 9200 Å) have some of the perturbing states as upper levels. This will be investigated later on.

An investigation of the perturbing matrix element reveals at a singlet-singlet interaction whether the perturbing state is a ${}^1\Pi$ or ${}^1\Sigma$ -state. At ${}^1\Sigma^1\Sigma$ perturbations the matrix element is independent of J , at ${}^1\Pi^1\Sigma$ perturbations it is proportional to $V/J(J+1)$. Only for one of the perturbations in CaO does such

an investigation give good information on the perturbing matrix element. The interaction studied is that at $J \sim 18$ in $v' = 2$. If δ_0 is the separation between the "unperturbed" terms and $(\delta_0 + 2\varepsilon)$ the separation between the perturbed terms, we have

$$\varepsilon(\varepsilon + \delta_0) = |H|^2.$$

ε and δ_0 may be determined as follows:

$$(2\varepsilon + \delta_0)J = R_1(J-1) - R_2(J-1) = P_1(J+1) - P_2(J+1)$$

and

$$\delta_0 = (B' - B_p)[J(J+1) - J_0(J_0+1)].$$

In the 2,0 and particularly in the 2,1 band these quantities are known over a range of J -values. For example, we have calculated 14 values of $|H|^2$ from the data of the 2,1 band. The determinations show that $|H|^2$ is independent of J and the calculated values do not alter systematically in any direction. The mean of these determinations is

$$|H|^2 = 285.$$

The maximal error in $|H|^2$ is 7, the mean error 1.0. The perturbing state is here X . If X is a singlet state it must be a $^1\Sigma$ -state. If X is a triplet state, it may be a $^3\Pi_0$ -substate, as the matrix element of $^3\Pi_0^1\Sigma$ interactions is independent of J .

Thus we can say the following: The upper state Σ^* is perturbed by six electronic states or substates X, Y, Z, Q, A and B . The first four have about the same B and ω -values (0.33 and 500 cm^{-1}). The last two have B and ω -values about 0.38 and 600 cm^{-1} . We cannot decide if any of the perturbing states are triplets or not. The matrix elements of $X\Sigma^*$ interactions are independent of J . If X is a singlet state, it is a $^1\Sigma$ -state.

§ 7. Determination of vibrational constants

Generally the vibrational constants are determined from the band-origins obtained from the relation

$$R(J-1) + P(J) = 2\nu_0 + 2(B' - B'')J^2 \quad (19)$$

and then by forming the differences $\Delta G(v + \frac{1}{2})$ for the upper and lower levels. In perturbed bands it is rather difficult, often impossible, to obtain ν_0 with any degree of accuracy.

In our case the lower levels are unperturbed and we can calculate very accurate vibrational constants for the lower state in the following way. Equ. (19) is written for two bands with the same upper level but with different lower levels (i and k),

$$[R(J-1) + P(J)]_{v', v'_i} = 2\nu_0(v', v'_i) + 2(B' - B'_i)J^2$$

$$[R(J-1) + P(J)]_{v', v'_k} = 2\nu_0(v', v'_k) + 2(B' - B'_k)J^2.$$

The difference between the equations — called A — is

$$A = 2[v_0(v', v'_i) - v_0(v', v'_k)] + 2(B''_k - B''_i)J^2 = 2[G''(v'_i) - G''(v'_k)] + \\ + 2(B''_k - B''_i)J^2. \quad (20)$$

Thus $G''(v'_i) - G''(v'_k)$ can be determined graphically from the relation (20). For CaO all possible combinations have been treated. ω''_e and $x''_e \omega''_e$ are computed from these equations by the method of least-squares. The constants obtained are

$$\omega''_e = 732.1_1 \\ x_e \omega''_e = 4.8_1.$$

It is more difficult to get good values for ω'_e and $x'_e \omega'_e$. In Table 2 the band-origins of all the analysed bands are given. The values are obtained from Equ. (19). We must, however, stress that, although the origins are determined from rotational levels seeming perturbed as little as possible, the values are very approximate. It is impossible to calculate the effect of the perturbations. Only for the X -perturbation in $v' = 2$ at $J \sim 18$ we could estimate this effect. The matrix-element for this perturbation is calculated ($|H|^2 = 285$). It is then possible to calculate the displacement ε for the perturbed upper rotational levels. We have

$$\varepsilon(\varepsilon + \delta_0) = 285$$

$$\delta_0 = (B'_2 - B_{x+3})[J(J+1) - J_0(J_0+1)] = 0.0772[J(J+1) - 342].$$

Before using Equ. (19), ε_J must be added to $R(J-1)$ and ε_{J-1} to $P(J)$. ε_J is determined for a range of J -values (24—40). For bands with $v' = 2$ in Table 2 the origins are given with this effect added. The correction is extremely great, namely about -5.5 cm^{-1} . This depends on the very large matrix element and on the fact that the perturbation culminates at a small J -value (18). It is not likely that any of the other interactions has such an effect on any origin, but it is not out of the question that some calculated origins are displaced by one or two units from their unperturbed positions. The vibrational constants for the upper state are approximately

$$\omega'_e = 716 \\ x'_e \omega'_e = 1.6.$$

§ 8. Results and comparison of CaO with the other alkaline earth oxides

Table 13 contains the most important data from this investigation. As in the case of the other alkaline earth oxides, it is most likely that the two $^1\Sigma$ -states are $^1\Sigma^+$ -states. It is, however, doubtful whether the lower state is the ground-state or not. There are, of course, some arguments in favour of this. The lower $^1\Sigma$ -state is unperturbed and the band-system very intense. The ground-state of the atoms O(^3P) and Ca(^1S) corresponds to a $^3\Sigma^-$ and a $^3\Pi$ -state only.

Table 13
Summary of Constants for CaO

State	$\nu_{0,0}$	ω_e	$x_e \omega_e$	B_e	α	D	$r_e \times 10^8 \text{ cm}$
$^1\Sigma^*$	11549	716	1.6	0.4063	0.0014 ₁	0.54×10^{-6}	1.906
Q	≤ 12238	~ 500	—	~ 0.33	—	—	~ 2.11
B	≤ 11748	~ 600	—	~ 0.38	—	—	~ 1.97
Y	≤ 11907	~ 500	~ 1.5	~ 0.33	0.001 ₅	—	~ 2.11
Z	≤ 11759	~ 500	~ 1.5	~ 0.33	0.001 ₅	—	~ 2.11
A	≤ 11650	~ 600	—	~ 0.38	—	—	~ 1.97
$X (^1\Sigma?)$	≤ 11549	~ 500	~ 1.5	~ 0.33	0.001 ₅	—	~ 2.11
$^1\Sigma$	0	732.1 ₁	4.8 ₁	0.4444 ₇	0.0033 ₅	0.658×10^{-6}	1.822

The lower $^1\Sigma$ -state must consequently dissociate into excited atoms. There are several possibilities here. It is remarkable that the lowest states — hitherto known, of all the alkaline earth oxides are $^1\Sigma^+$ -states.

If the dissociation energies are calculated from the formula $D = \omega^2/4x\omega$ we obtain

$$D'' = 3.5, \quad D' = 9.9.$$

These values are of course very approximate, especially that for D' .

Comparing the vibrational constants derived in this investigation with constants for other systems obtained by other authors, we notice that MAHANTI has given about the same constants for the upper state of the blue bands and the lower state of the ultra-violet bands as we have calculated for our lowest state. MAHANTI's head-equations are:

$$\begin{aligned} \text{Blue bands: } \nu_h &= 23,817.62 + 726.53 (v' + \tfrac{1}{2}) - 11.66 (v' + \tfrac{1}{2})^2 \\ &\quad - 811.28 (v'' + \tfrac{1}{2}) - 6.60 (v'' + \tfrac{1}{2})^2 \end{aligned}$$

$$\begin{aligned} \text{Ultra-violet bands: } \nu_h &= 24,702.81 + 565.06 (v' + \tfrac{1}{2}) - 4.48 (v' + \tfrac{1}{2})^2 - \\ &\quad - 725.37 (v'' + \tfrac{1}{2}) - 3.56 (v + \tfrac{1}{2})^2. \end{aligned}$$

Especially the constants for the lower state of the ultra-violet bands agree rather well. The constant $x'\omega' = 11.66$ for the blue bands seems very high. LEJEUNE and ROSEN have also reported ω -values of the magnitude 600—700 cm^{-1} . As we have not investigated any other band-systems in CaO than the infra-red $^1\Sigma^* - ^1\Sigma$ transition, we shall refrain here from any discussion of the term scheme. Such a discussion can only be fruitful after reliable rotational analyses of the other systems.

As has already been mentioned, the lowest states of the alkaline earth oxides are all $^1\Sigma^+$ -states. The B_e -values, ω_e -values, force-constants and internuclear distances are given in Table 14. It is noteworthy that the force-constants vary in a very unexpected way. This may indicate that some of the $^1\Sigma^+$ -states given in Table 14 are not the ground-states. The internuclear distances vary very regularly. It is, however, likely that the force-constants are more sensitive to variation in the bond type than are the internuclear distances.

Table 14

B_e -values, ω_e -values, force-constants (K_e'') and internuclear distances for the lowest states of the alkaline earth oxides

Molecule	B_e	ω_e	K_e''	r_e''	Reference
BeO	1.6510	1487	7.52×10^5 dynes/cm	1.33×10^{-8}	LAGERQVIST a. WESTÖÖ (1945)
MgO	0.5743	785	3.46	1.75	LAGERQVIST a. UHLER (1949)
CaO	0.4445	732	3.61	1.82	ALMKVIST a. LAGERQVIST (1950)
SrO	0.3378	653	3.40	1.92	
BaO	0.3125	670	3.79	1.94	BARROW, LAGERQVIST, LIND (1950)

We hope later on to be able to treat the blue and the ultra-violet bands and the band-systems situated in the far infra-red.

We should like to express our gratitude to Professor E. HULTHÉN for his keen interest.

April, 1950. Physics Department, The University, Stockholm.

REFERENCES. Almkvist, G. and Lagerqvist, A., 1949, Arkiv för Fysik, 1, 477. — —, 1950, Arkiv för Fysik, 2, 233. — Barrow, R., Lagerqvist, A. and Lind, E., 1950, Proc. Phys. Soc., 63 A, 1132. — Brodersen, P. H., 1932, Z. Physik, 79, 613. — —, 1936, Z. Physik, 104, 135. — Gerö, L., 1935, Z. Physik, 93, 669. — King, A. S., 1908, Astrophys. Jour. 27, 353. — Kovács, I., 1937 a, Z. Physik, 106, 431. — —, 1937 b, Inaugural Dissertation, Budapest. — Kovács, I. and Lagerqvist, A., 1950, Arkiv för Fysik, 2, 411. — Kovács, I. and Singer, S., 1942, Phys. Z., 43, 362. — Lagerqvist, A. and Uhler, U., 1949, Arkiv för Fysik, 1, 459. — Lagerqvist, A. and Westöö, R., 1945, Ark. Mat. Astr. o. Fys. 32 A, No. 10. — Lejeune, J.-M. and Rosen, B., 1945, Bull. Soc. Roy. Sci. Liège, 322. — Mahanti, P. C., 1932, Phys. Rev., 46, 268. — Mahla, K., 1933, Z. Physik, 81, 625. — Meggers, W. F., 1933, Bur. of Stand., 10, 669. — M. I. T. Wave-length Tables, 1939. (Chapman and Hall: London).

Tryckt den 18 januari 1951

Uppsala 1951. Almqvist & Wiksells Boktryckeri AB

